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Slemrod's research in 1990-91 centered on two issues: (1) the kinetics of coagulation processes, (2) behavior of discrete velocity models in the kinetic theory of gases. In the first area Selmrod has (a) given a new method for solving the special class of coagulation equations which exhibit gelation and (b) derived and proved existences of similarilty solutions for coagulation equations with diffusion. In the second area Slemrod has used his "relaxed invariance principle" method to prove weak decay to equilibrium for the Braodwell model of gas dynamics in the case of specularly reflective boundary conditions.

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FINAL TECHNICAL REPORT

Problems in Nonlinear Continuum Dynamics

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Summary

Slemrod's research in 1990-91 centered on two issues: (1) the kinetics of coagulation processes, (2) behavior of discrete velocity models in the kinetic theory of gases. In the first area Slemrod has (a) given a new method for solving the special class of coagulation equations which exhibit gelation and (b) derived and proved existence of similarity solutions for coagulation equations with diffusion. In the second area Slemrod has used his "relaxed invariance principle" method to prove weak decay to equilibrium for the Broadwell model of gas dynamics in the case of specularly reflective boundary conditions.

In the last year Slemrod's research has centered on two issues: (1) the kinetics of coagulation processes, (2) behavior of discrete velocity models in kinetic theory of gases. Below an outline of progress in each area is given.

1. Kinetics of Coagulation Processes

Models of cluster growth appear in a wide variety of applications. One well known example is the Smoluchowski-Flory-Stockmayer theory of gelation where it was found that all concentrations decrease in time and the quantity representing mass density is conserved for only a finite time after which it decreases.

The models themselves are coupled infinite systems of ordinary differential equations: Let $c_j(t) \geq 0$, $j = 1, 2, \ldots$ denote the expected numbers of clusters consisting of j particles per unit volume. The discrete coagulation-fragmentation equations are

$$\begin{aligned} \frac{dc_j}{dt} &= \frac{1}{2}\sum_{k=1}^{j-1}[a_{j-k,k}c_{j-k}c_k - b_{j-k,k}c_j] \\ &\quad - \sum_{k=1}^{\infty}[a_{j,k}c_jc_k - b_{j,k}c_{j+k}] \quad \text{for} \quad j = 1, 2\ldots \end{aligned} \tag{1}$$

The coagulation rate $a_{j,k}$ and fragmentation rate $b_{j,k}$ are non-negative constants with $a_{j,k} = a_{k,j}$, $b_{j,k} = b_{k,j}$.

In paper [1], Slemrod considered *the case of pure coagulation for which* $b_{jk} \equiv 0$ *and the* special case $a_{jk} = jk$. In this case the Smoluchowski-Flory-Stockmayer system becomes

$$\frac{dc_j}{dt} = \frac{1}{2}\sum_{k=1}^{j-1}(j-k)kc_{j-k}c_k - jc_j\sum_{k=1}^{\infty}kc_k\,. \tag{2}$$

For simplicity monodisperse initial data was chosen $c_1(0) = 1$, $c_j(0) = 0$, $2 \leq j < \infty$.

A solution of (2) has been given by McLeod (J. B. McLeod, On an infinite set of non-linear differential equations, Quarterly J. Math. Oxford Ser (2), 13 (1962), 119-128). McLeod's solution was valid on $0 \leq t \leq 1$. It was based on the fact that on $0 \leq t \leq 1$ the mass density $\rho(t) = \sum_{k=1}^{\infty} kc_k(t)$ is conserved (and equals one). However as McLeod noted the desired conservation of density breaks down for $t > 1$ and his solution is not valid past the critical "gelation" *time*, $t = 1$.

The first resolution of the problem was provided by Leyvraz and Tschudi (F. Leyvraz and H. R. Tschudi, Singularities in the kinetics of coagulation processes, J. Phys. A. 14 (1981), 3389-3405). Their method was to introduce the generating function $G(z,t) = \sum_{k=1}^{\infty}\phi_k(t)z^k$ where $\phi_j(t) = jc_j(t)\exp(j\int_0^t \rho(z)dz)$. A computation shows G satisfies the quasi-linear hyperbolic partial differential equation

$$\frac{\partial G}{\partial t} = zG\frac{\partial G}{\partial z} \qquad 0 \leq z \leq 1,\, t > 0 \tag{3}$$

with initial data $G(z,0) = z$. They integrated (3) via the method of characteristics and then recovered $c_j(t)$. The end result (after long computations) was that

$$
\begin{aligned}
c_j(t) &= \frac{j^{j-3}e^{-j}}{(j-1)!}\frac{1}{t} \qquad t \geq 1 \\
&= \frac{j^{j-3}t^{j-1}}{(j-1)!}e^{-jt} \qquad 0 \leq t \leq 1 .
\end{aligned}
\tag{4}
$$

In this case the density $\rho(t)$ satisfies

$$
\begin{aligned}
\rho(t) &= 1 \qquad 0 \leq t \leq 1 \\
&= \frac{1}{t} \qquad 1 \leq t < \infty
\end{aligned}
\tag{5}
$$

indicating a decrease in density after the "gelation" time $t = 1$.

In [1] Slemrod reconsidered resolution (2) based on McLeod's original ideas with some subtle changes. He was able to show the density $\rho(t)$ satisfies the singular ordinary differential equation

$$
\left(\frac{1}{\rho(t)} - t\right)\frac{d\rho}{dt}(t) = 0 , \qquad \rho(0) = 1 \tag{6}
$$

which immediately yields (5) and thus (4). Hence no recourse to complicated use of characteristics and generating functions is needed and a clear picture of the evolution of the density is provided.

In a second paper Slemrod [2] following ideas of Binder (K. Binder, Theory for the dynamics of clusters, II. *Critical diffusion in binary systems* and the kinetics of phase separation, Phys. Rev. B 15 (1977), 4425-4447), considered the incorporation of diffusion in the classical discrete coagulation-fragmentation system (1). Again the restriction was made to pure coagulation ($b_{jk} \equiv 0$) but now the added difficulty of diffusion (as given by Stokes' law) is considered.

The equations now are for quantities $c_j(\underline{x}, t) \geq 0$, $j = 1, 2...$ which denote the expected number of clusters of j particles/unit volume at position $\underline{x} \in \mathbb{R}^n (n = 1, 2, 3)$ at time $t \geq 0$. The discrete coagulation-diffusion equations are

$$
\begin{aligned}
\frac{\partial c_j}{\partial t} - D_j \Delta c_j = \frac{1}{2}\sum_{k=1}^{j-1} a_{j-k,k}c_{j-k}c_k - \sum_{k=1}^{\infty} a_{j,k}c_jc_k , \\
j = 1, 2, ... ;
\end{aligned}
\tag{7}
$$

$D_j \sim j^{-1/n}$ (Stokes' law).

In [2] Slemrod considered a variety of problems: Existence of steady states, finite time gelation, and diffuse interfaces. A particularly interesting point is that system (7) admits an exact similarity form $c_j(R, t) = \phi_j(\xi)/t$ where $\xi = R/\sqrt{t}$, $R = |\underline{x}|$. The functions $\phi_j(\xi)$ satisfy the infinite systems of ordinary differential equations

$$
\begin{aligned}
D_j(\phi_j'' + \frac{n-1}{\xi}\phi_j') + \frac{1}{2}\xi\phi_j' + \phi_j = \\
= -\frac{1}{2}\sum_{k=1}^{j-1} a_{j-k,k}\phi_{j-k}\phi_k + c_j \sum_{k=1}^{\infty} a_{j,k}\phi_j\phi_k .
\end{aligned}
\tag{8}
$$

In [2] Slemrod also provided some preliminary existence theorems for solvability of (8).

2. Discrete Velocity Models of Gases

Discrete velocity models are finite velocity approximations of the Boltzmann equation. They provide a mathematical simplification for the true Boltzmann equation hence often allowing more complete analysis than can presently be done for the true Boltzmann equation. One such discrete velocity model is the Broadwell model which describes a gas of particles with identical masses moving along three perpendicular coordinates with same speed c. Results of a particular collision have the same probability with only binary collisions allowed. Let $N_i = N_i(x,y,z,t)$, $i = 1,2,...,6$, denote the density of particles moving in the six allowed directions. Then $N_1,...,N_6$ satisfy the Broadwell system

$$\begin{aligned}
\frac{\partial N_1}{\partial t} + c\frac{\partial N_1}{\partial x} &= \sigma(N_3N_4 + N_5N_6 - 2N_1N_2)\,,\\
\frac{\partial N_2}{\partial t} - c\frac{\partial N_2}{\partial x} &= \sigma(N_3N_4 + N_5N_6 - 2N_1N_2)\,,\\
\frac{\partial N_3}{\partial t} + c\frac{\partial N_3}{\partial y} &= \sigma(N_1N_2 + N_5N_6 - 2N_3N_4)\,,\\
\frac{\partial N_4}{\partial t} - c\frac{\partial N_4}{\partial y} &= \sigma(N_1N_2 + N_5N_6 - 2N_3N_4)\,,\\
\frac{\partial N_5}{\partial t} + c\frac{\partial N_5}{\partial z} &= \sigma(N_1N_2 + N_3N_4 - 2N_5N_6)\,,\\
\frac{\partial N_6}{\partial t} - c\frac{\partial N_6}{\partial z} &= \sigma(N_1N_2 + N_3N_4 - 2N_5N_6)\,,
\end{aligned} \tag{9}$$

where $\sigma/2c$ is the cross section for binary collisions.

For flows which are independent of y, z and for which $N_3 = N_4 = N_5 = N_6$ the above six velocity model reduces to the simpler form

$$\begin{aligned}
\frac{\partial N_1}{\partial t} + c\frac{\partial N_1}{\partial x} &= 2\sigma(N_3^2 - N_1N_2)\,,\\
\frac{\partial N_2}{\partial t} - c\frac{\partial N_2}{\partial x} &= 2\sigma(N_3^2 - N_1N_2)\,,\\
\frac{\partial N_3}{\partial t} &= \sigma(N_1N_2 - N_3^2)\,.
\end{aligned} \tag{10}$$

An open problem concerning (10) has been the asymptotic behavior (as $t \to \infty$) of (10) with initial conditions

$$N_1(x,0) = N_{10}(x),\ N_2(x,0) = N_{20}(x),\ N_3(x,0) = N_{30}(x),\ 0 < x < 1 \tag{11}$$

and boundary conditions of specular reflection type

$$N_1(x,t) = N_2(x,t) \quad \text{for} \quad t > 0, \quad x = 0,1\,. \tag{12}$$

In [3] Slemrod gave a resolution fo this problem via his "relaxed" invariance principle based on dynamical systems in infinite dimensional state spaces and Young measures. The main result is that as $t \to \infty$ the unique solution of (10), (11), (12) tends to traveling waves $f_1(x-ct)$, $f_2(x+ct)$, $f_3(x)$ satisfying the collision inequality

$$f_1(x-ct)\, f_2(x+ct) \leq f_3(x)^2 \quad \text{a.e.} \quad x \,\epsilon\, [0,1],\, t \geq 0\,.$$

Convergence to $f_1(x-ct)$, $f_2(x+ct)$, $f_3(x)$ is in the weak* topology of an appropriate $L_1 log L_1$ Banach space.

Publications

1. M. Slemrod, A Note on the Kinetic Equations of Coagulation, J. Integral Eqns and Applic. Vol 3 Number 1, Winter 1991, 167-173.
2. M. Slemrod, Coagulation-Diffusion Systems: Derivation and Existence of Solutions for the Diffuse Interface Structure Equations, Physica D 46 (1990), 351-366.
3. M. Slemrod, Large Time Behavior of the Broadwell Model of a Discrete Velocity Gas with Specularly Reflective Boundary Conditions, Arch. Rational Mech. and Analysis, Vol 111, Number 4 (1990), 323-342.